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FINAL REPORT

Nonlinear Effects in High Electric Fields

H.J. Kreuzer, Department of Physics
Dalhousie University, Halifax, N.S. B3H 3J5, Canada

Research results have been reported in two previous year-end reports in 1991 and 1992, respectively. The highlights from those reports, and developments since, are as follows:

(1) We have completed a first principles calculation of the field adsorption of metals on metals, Technical Report #5. We found in particular a field enhancement above single atoms on an otherwise flat metal surface (jellium) by up to a factor of 2. This is a crucial piece of information to understand the high ionizaiton rates in the field ion microscope above protruding atoms. Experiments to verify our theoretical predictions have been performed at the Fritz-Haber-Institute, see Technical report #12.

(2) The density functional calculations of field adsorption of rare gases on metals have been completed with first results in Technical Report #11. A comprehensive article, written together with R.G. Forbes of the University of Surrey, is in its final stages. There we draw together the insights from earlier classical models and from our quantum mechanical calculations to get a unified picture of field enhancement and field-induced chemisorption.

(3) Field adsorption of various hydrogen species on metals has been studied both theoretically in my group and in collaboration with Block's experimental group at the Fritz-Haber-Institut in Berlin. A recent topic was thermal field desorption of hydrogen for which we have been able to explain binding characteristics and energy distributions, the latter based on a second order kinetic model, see Technical Report #13.

(4) The work on Metal Clusters in Electric Fields, mentioned in the 1992 year-end report is being continued. We have so far generalized the earlier, spherical model to a spheroidal model to include coupling of different multipolar fields. This topic is also the subject of a new grant from ONR.

Publications

1. L.C. Wang and H.J. Kreuzer. Kinetic Theory of Field Evaporation of Metals. Surface Sci. **237**, 337-346 (1990). (Technical Report #1)

2. H.J. Kreuzer and L.C. Wang. Field-Induced Surface Chemistry of NO. J. Chem. Phys. **93**, 6065-6069 (1990). (Technical Report #2)

3. H.J. Kreuzer. Physics and Chemistry in High Eletric Fields. (Invited talk, 37th International Field Emission Symposium, Albuquerque, NM, July 30 August 3, 1990) Surface Sci. **246**, 336-347 (1991). (Technical Report #3)

4. J.H. Block, H.J. Kreuzer, and L.C. Wang. Electrostatic Field Effects in Surface Reactivity: Adsorption, Dissociation and Catalytic Reaction of Nitric Oxide. Surface Sci. **246**, 125-134 (1991). (Technical Report #4)

5. H.J. Kreuzer, L.C. Wang, and N.D. Lang. Self-Consistent Calculation of Atomic Adsorption on Metals in High Electric Fields. Phys. Rev *B* **45**, 12050-12055 (1992). (Technical Report #5)

6. Zhi *Xu*, J.T. Yates, Jr., L.C. Wang, and H.J. Kreuzer. Chemisorbed CO Site Interconversion on *Ni*(111) Induced by the Electric Field of Physisorbed Second Layers. J. Chem. Phys. **96**, 1628-1635 (1992). (Technical Report #6)

7. H.J. Kreuzer. Chemical Reactions in High Electric Fields. (Invited Talk, ACS Meeting, Atlanta, GA, April 15-18,1991). In *Surface Science of Catalysis: In-Situ Probes and Reaction Kinetics*, eds. D.J. Dwyer and F.M. Hoffmann, ACS Symposium Series, vol. **482** (American Chemical Society, Washington, 1992) *pp*. 268-286. (Technical Report #7)

8. U. Dürig, O. Züger, L.C. Wang, and H.J. Kreuzer. Adhesion in Atomic Scale Metal Contacts. Europhysics Letters (submitted). (Technical Report #8)

9. Xiaoming *Ye*, H.J. Kreuzer , and D.R. Salahub. Theory of Field Adsorption of Hydrogen. Applied Surface Science **67** (1993) 1-8. (Technical Report #9)

10. H.J. Kreuzer. Physics and Chemistry in High Electric Fields. (Invited Talk, International Conference on Atomic and Nanoscale Modification of Materials: Fundamentals and Applications, Ventura, California, August 16-21, 1992) In *Atomic and Nanoscale Modification of Materials: Fundamentals and Applications*, Ed. Ph. Avouris, NATO-ASI-*E* Series "Applied Science" (Kluwer Academic Publishers, 1993). (Technical Report #10)

11. H.J. Kreuzer and R.L.C. Wang. Physics and Chemistry in High Electric Fields. (Invited Talk, Conference on Density Functional Theory and its Applications, Oxford, England, September 16-18, 1992). Philosophical Magazine, Part *B*. (Technical Report #11)

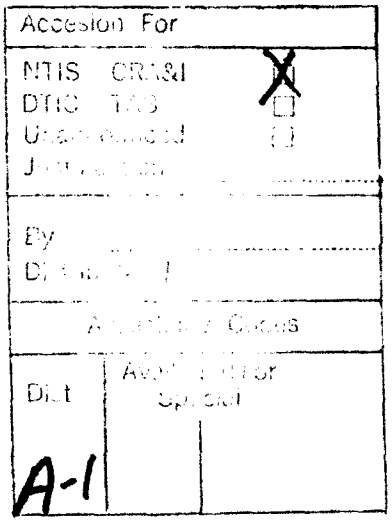
12. Yu. Suchorski, W.A. Schmidt, J.H. Block, and H.J. Kreuzer. Compari-

tive Studies on Field Ionization at Surface Sites of *Rh*, *Ag*, and Au: Differences in Local Electric Field Enhancement. Surface Science (submitted). (Technical Report #12)

13. N. Ernst, J.H. Block, H.J. Kreuzer, and Xiaoming Ye. Thermal Field Desorption Spectroscopy of Molecular Hydrogen Ions. Physical Review Letters (submitted). (Technical Report #13)

Personnel paid from this grant:

(1) Dr. R.L.C. Wang, Research Associate
(2) Xiaoming Ye, Graduate student (obtained his Phd in June 1992.
(3) H.J. Kreuzer, teaching release time.
(4) Summer students: M. Crawford, A. Hare, B. Hughes
(5) Visitors: Prof. J.H. Block, Dr. N. Ernst.



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Physics and Chemistry in High Electric Fields

by

H. J. Kreuzer and R. L. C. Wang

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Department of Physics, Dalhousie University
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H. J. Kreuzer and R. L. C. Wang

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Dalhousie University, Department of Physics
Halifax, N.S.
Canada B3H 3J5

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U.S.A.

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Progress is reviewed in our understanding of the effects of high electrostatic fields (of the order of volts per angstrom) on the adsorption and reaction of atoms and molecules on metal surfaces.

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Technical Report No. 12

Comparative Studies on Field Ionization at Surface Sites of Rh, Ag, and Au: Differences in Local Electric Field Enhancement

by

Yu. Suchorski[1], W. A. Schmidt[1], J. H. Block[1]
and
H. J. Kreuzer[2]

To be published in

Surface Science

[1]Fitz-Haber Institut der Max-Planck-Gesellschaft
Fradayweg 4-6, 1000 Berlin 33, Germany
and
[2]Department of Physics, Dalhousie University
Halifax, Nova Scotia, Canada B3H 3J5

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Yu. Suchorski, W. A. Schmidt, J. H. Block and H. J. Kreuzer

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Dalhousie University, Department of Physics
Halifax, N.S.
Canada B3H 3J5

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Office of Naval Research
800 N. Quincy Street
Arlington, VA 22217-5000
U.S.A.

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Field ion imaging conditions were studied for clean Rh, and for Rh expitaxially covered with Ag, and Au, respectively. Significant, metal-specific decreases of the image voltages have been observed. This is casued by different enhancements of local fields in the vicinity of protruding Rh, Ag and Au atoms due to their different electronic structures. The interpretation is based on self-consistent calculations of local electrostatic field distributions in the vicinity of single atoms adsorbed on a metal surface. For different facets on a surface, a close correlation between local field distributions and the degree of localization of the field ionization process is established from measured FWHM on field ion energy distributions and is discussed in association with possible field ionization mechanisms.

14. SUBJECT TERMS
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Technical Report No. 13

Thermal Field Desorption Spectroscopy of Chemisorbed Hydrogen for a Single Step Site

by

N. Ernst[1], J. H. Block[1], H. J. Kreuzer[2] and X. Ye[2]

Submitted to

Physical Review Letters

[1]Fitz-Haber Institut der Max-Planck-Gesellschaft
Fradayweg 4-6, 1000 Berlin 33, Germany
and
[2]Department of Physics, Dalhousie University
Halifax, Nova Scotia, Canada B3H 3J5

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Dalhousie University, Department of Physics
Halifax, N.S.
Canada B3H 3J5

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13. ABSTRACT (Maximum 200 words)

The molecular hydrogen ion yield from a single atomic step site of a [100]-oriented tungsten and of a [100]-oriented rhodium crystal is determined as a function of surface temperature using mass and energy resolved probe hole field ion microscopy. A second order kinetic model is developed to fit the experimental data thus obtaining the hydrogen binding energy. For local fields of about 3 V/Å the data is close to values obtained from thermal desorption spectroscopy. A comparison is made with calculations of the field-absorption binding energy of atomic hydrogen on a jellium surface based on density functional theory.

14. SUBJECT TERMS
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